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## Structure Reports

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**(E)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one****Pei-Hua Zhao,<sup>a\*</sup> Er-Jun Hao,<sup>b</sup> Ya-Qing Liu<sup>a</sup> and Gui-Zhe Zhao<sup>a</sup>**

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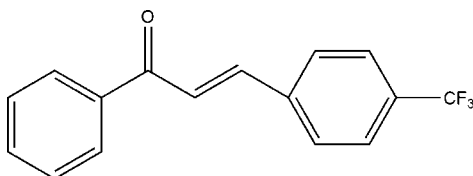
Received 13 March 2012; accepted 14 August 2012

Key indicators: single-crystal X-ray study;  $T = 113$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.078; data-to-parameter ratio = 16.6.

In the title compound,  $\text{C}_{16}\text{H}_{11}\text{F}_3\text{O}$ , the dihedral angle between the two rings is  $48.8(2)^\circ$ . The crystal packing exhibits no classical intermolecular interactions between the molecules.

**Related literature**

For applications of related compounds, see: Shibata (1994); Devincenzo *et al.* (1995); Dimmock *et al.* (1999); Go *et al.* (2005).

**Experimental***Crystal data* $\text{C}_{16}\text{H}_{11}\text{F}_3\text{O}$  $M_r = 276.25$ 

Monoclinic,  $P2_1/c$   
 $a = 14.7469(5)$  Å  
 $b = 14.5697(4)$  Å  
 $c = 5.8430(2)$  Å  
 $\beta = 92.854(1)^\circ$   
 $V = 1253.86(7)$  Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 113$  K  
 $0.20 \times 0.18 \times 0.08$  mm

*Data collection*

Rigaku Saturn724 CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku/MS, 2005)  
 $T_{\min} = 0.976$ ,  $T_{\max} = 0.990$

12984 measured reflections  
 3005 independent reflections  
 2037 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.078$   
 $S = 1.12$   
 3005 reflections

181 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.27$  e Å<sup>-3</sup>

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MS, 2005).

This work was supported financially by the National Natural Science Foundation of China (No. 51102216) and Shanxi Province Science Foundation for Youths (No. 2012021007-4).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2055).

**References**

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## supplementary materials

*Acta Cryst.* (2012). E68, o2750 [doi:10.1107/S1600536812035763]

**(E)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one**

Pei-Hua Zhao, Er-Jun Hao, Ya-Qing Liu and Gui-Zhe Zhao

**Comment**

The title compound belongs to the chalcones, which are Michael acceptors and constitute an important group of natural products that belong to the flavonoid family (Dimmock *et al.*, 1999; Go *et al.*, 2005). Natural and synthetic chalcones have been reported to possess strong antiproliferative effects in ovarian cancer cells and in gastric cancer cells (Shibata, 1994; Devincenzo *et al.*, 1995).

The dihedral angle between two benzene rings is 48.8 (2) ° (Fig. 1). The crystal packing shows no  $\pi\cdots\pi$  or other classical intermolecular interactions (Fig. 2).

**Experimental**

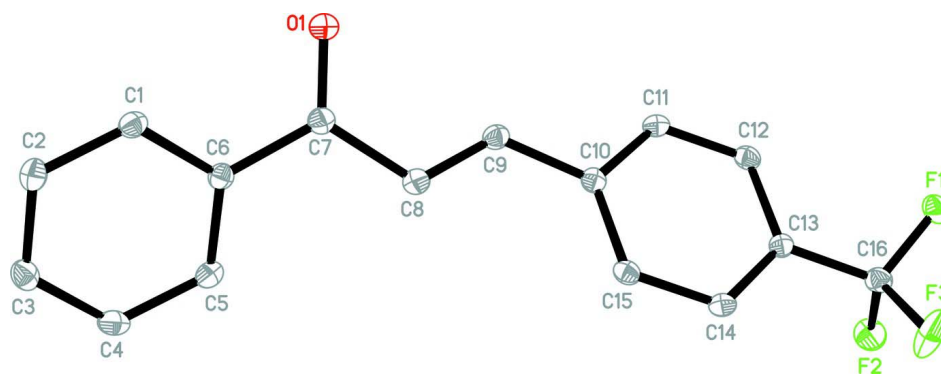
In 25 ml round-bottomed flask, the acetophenone (5.0 mmol) and sodium hydroxide (7.5 mmol) were dissolved in ethanol (2 ml), and the mixture was stirred at room temperature for 5 min followed by addition of 4-trifluoromethylbenzaldehyde (5.0 mmol). The reaction mixture was then stirred at room temperature and monitored by TLC until the reaction completed. The solid was filtered, washed with cold water, recrystallized from ethanol, and dried *in vacuo* to give the desired product. Crystals of the title compound were obtained by slow evaporation of the dichloromethane/*n*-hexane solution (1:1) at room temperature. <sup>1</sup>N NMR(400 MHz, CDCl<sub>3</sub>, TMS): 7.53 (dd, 2H, J = 7.6, 15.6 Hz), 7.60 (m, 2H), 7.68 (d, 2H, J = 8.0 Hz), 7.75 (d, 2H, J = 8.0 Hz), 7.82 (d, 1H, J = 15.6 Hz), 8.03 (d, 2H, J = 8.4 Hz) p.p.m..

**Refinement**

All the H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

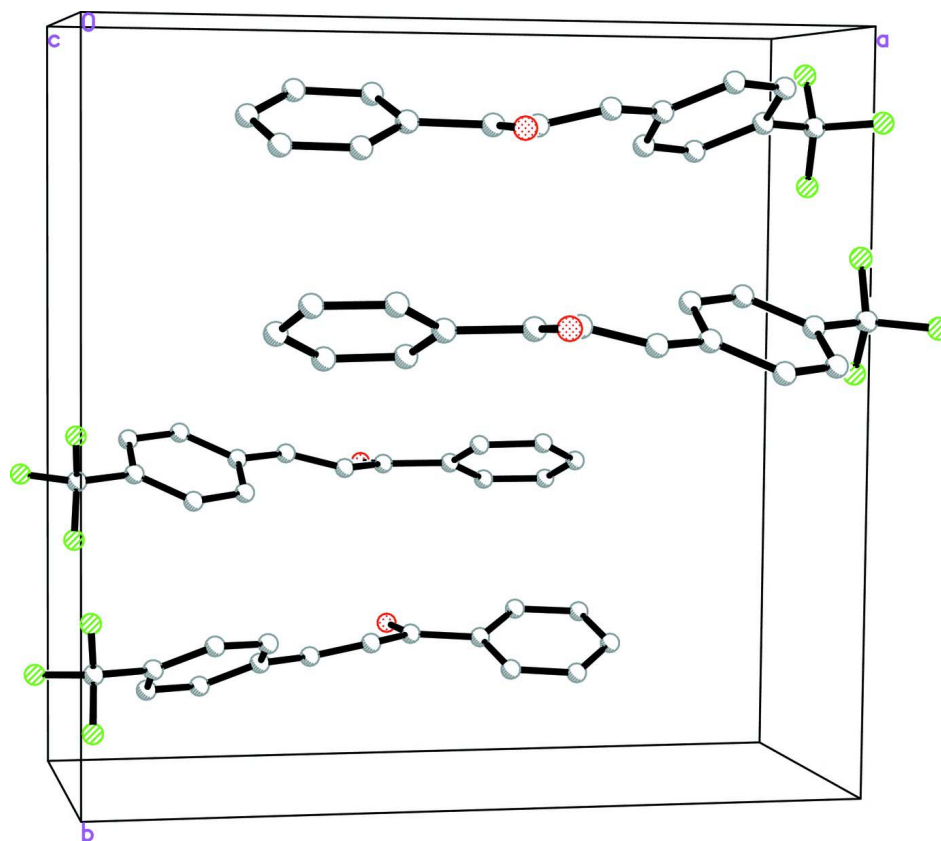
**Computing details**

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear* (Rigaku/MSC, 2005); data reduction: *CrystalClear* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).



**Figure 1**

The molecular structure of the title compound. Thermal displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted.



**Figure 2**

The crystal packing of the title compound.

**(E)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one**

*Crystal data*

$C_{16}H_{11}F_3O$

$M_r = 276.25$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 14.7469\ (5)\ \text{\AA}$

$b = 14.5697\ (4)\ \text{\AA}$

$c = 5.8430\ (2)\ \text{\AA}$

$\beta = 92.854\ (1)^\circ$

$V = 1253.86 (7) \text{ \AA}^3$   
 $Z = 4$   
 $F(000) = 568$   
 $D_x = 1.463 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
Cell parameters from 4102 reflections

$\theta = 2.0\text{--}28.0^\circ$   
 $\mu = 0.12 \text{ mm}^{-1}$   
 $T = 113 \text{ K}$   
Prism, colorless  
 $0.20 \times 0.18 \times 0.08 \text{ mm}$

#### Data collection

Rigaku Saturn724 CCD  
diffractometer  
Radiation source: rotating anode  
Multilayer monochromator  
Detector resolution:  $14.22 \text{ pixels mm}^{-1}$   
 $\omega$  and  $\phi$  scans  
Absorption correction: multi-scan  
(*CrystalClear*; Rigaku/MSO, 2005)  
 $T_{\min} = 0.976$ ,  $T_{\max} = 0.990$

12984 measured reflections  
3005 independent reflections  
2037 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$   
 $\theta_{\max} = 27.9^\circ$ ,  $\theta_{\min} = 2.0^\circ$   
 $h = -19 \rightarrow 19$   
 $k = -14 \rightarrow 19$   
 $l = -7 \rightarrow 7$

#### Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.078$   
 $S = 1.12$   
3005 reflections  
181 parameters  
0 restraints  
Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map  
Hydrogen site location: inferred from  
neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0283P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.27 \text{ e \AA}^{-3}$

#### Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

#### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	1.01951 (5)	0.12265 (5)	1.04772 (13)	0.0377 (2)
F2	0.95432 (5)	0.05980 (5)	1.32422 (13)	0.0375 (2)
F3	0.95565 (5)	0.20580 (5)	1.29461 (15)	0.0493 (3)
O1	0.47484 (6)	0.13892 (6)	0.27878 (15)	0.0329 (2)
C1	0.29314 (8)	0.16320 (7)	0.3888 (2)	0.0215 (3)
H1	0.3095	0.1866	0.2449	0.026*
C2	0.20299 (9)	0.16081 (7)	0.4417 (2)	0.0243 (3)
H2	0.1576	0.1834	0.3353	0.029*
C3	0.17888 (9)	0.12555 (8)	0.6496 (2)	0.0249 (3)
H3	0.1168	0.1235	0.6851	0.030*
C4	0.24500 (8)	0.09312 (8)	0.8068 (2)	0.0251 (3)

H4	0.2280	0.0684	0.9489	0.030*
C5	0.33571 (8)	0.09691 (8)	0.7565 (2)	0.0225 (3)
H5	0.3811	0.0761	0.8655	0.027*
C6	0.36044 (8)	0.13127 (7)	0.5461 (2)	0.0198 (3)
C7	0.45675 (8)	0.13432 (8)	0.4807 (2)	0.0220 (3)
C8	0.52985 (8)	0.13323 (8)	0.6661 (2)	0.0230 (3)
H8	0.5162	0.1474	0.8193	0.028*
C9	0.61401 (8)	0.11232 (7)	0.6158 (2)	0.0207 (3)
H9	0.6223	0.0939	0.4623	0.025*
C10	0.69610 (8)	0.11424 (7)	0.7696 (2)	0.0188 (3)
C11	0.77584 (8)	0.07768 (7)	0.6888 (2)	0.0202 (3)
H11	0.7745	0.0490	0.5426	0.024*
C12	0.85708 (8)	0.08253 (8)	0.8182 (2)	0.0211 (3)
H12	0.9109	0.0571	0.7615	0.025*
C13	0.85929 (8)	0.12479 (7)	1.0312 (2)	0.0185 (3)
C14	0.78038 (8)	0.16112 (7)	1.1158 (2)	0.0202 (3)
H14	0.7820	0.1899	1.2619	0.024*
C15	0.69934 (8)	0.15519 (7)	0.9860 (2)	0.0205 (3)
H15	0.6453	0.1793	1.0449	0.025*
C16	0.94629 (8)	0.12902 (8)	1.1725 (2)	0.0234 (3)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0177 (4)	0.0663 (5)	0.0293 (5)	−0.0017 (4)	0.0027 (3)	0.0043 (4)
F2	0.0314 (5)	0.0496 (5)	0.0311 (5)	0.0037 (3)	−0.0037 (4)	0.0171 (4)
F3	0.0378 (5)	0.0427 (5)	0.0648 (6)	0.0105 (4)	−0.0231 (5)	−0.0281 (4)
O1	0.0250 (5)	0.0531 (6)	0.0208 (5)	−0.0003 (4)	0.0020 (4)	0.0019 (4)
C1	0.0247 (7)	0.0216 (6)	0.0180 (7)	−0.0040 (5)	−0.0002 (5)	0.0000 (5)
C2	0.0216 (7)	0.0227 (7)	0.0282 (8)	−0.0008 (5)	−0.0028 (6)	−0.0013 (5)
C3	0.0217 (7)	0.0240 (7)	0.0291 (7)	−0.0045 (5)	0.0044 (6)	−0.0065 (6)
C4	0.0313 (7)	0.0248 (7)	0.0198 (7)	−0.0074 (6)	0.0059 (6)	−0.0031 (5)
C5	0.0254 (7)	0.0224 (6)	0.0193 (7)	−0.0015 (5)	−0.0023 (5)	0.0004 (5)
C6	0.0206 (6)	0.0190 (6)	0.0198 (7)	−0.0023 (5)	0.0000 (5)	−0.0023 (5)
C7	0.0222 (7)	0.0229 (6)	0.0209 (7)	0.0002 (5)	0.0010 (5)	0.0009 (5)
C8	0.0234 (7)	0.0259 (7)	0.0197 (7)	−0.0017 (5)	0.0008 (5)	−0.0011 (5)
C9	0.0239 (7)	0.0195 (6)	0.0188 (7)	−0.0013 (5)	0.0008 (5)	−0.0010 (5)
C10	0.0206 (6)	0.0157 (6)	0.0201 (7)	−0.0012 (5)	0.0013 (5)	0.0026 (5)
C11	0.0248 (7)	0.0194 (6)	0.0165 (6)	0.0011 (5)	0.0025 (5)	−0.0007 (5)
C12	0.0201 (6)	0.0223 (6)	0.0211 (7)	0.0033 (5)	0.0042 (5)	0.0007 (5)
C13	0.0197 (6)	0.0174 (6)	0.0183 (6)	0.0006 (5)	0.0003 (5)	0.0029 (5)
C14	0.0238 (7)	0.0199 (6)	0.0170 (6)	0.0020 (5)	0.0020 (5)	−0.0013 (5)
C15	0.0199 (7)	0.0208 (6)	0.0211 (7)	0.0031 (5)	0.0048 (5)	0.0005 (5)
C16	0.0224 (7)	0.0255 (7)	0.0226 (7)	0.0032 (5)	0.0027 (5)	−0.0010 (6)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

F1—C16	1.3361 (14)	C7—C8	1.4896 (16)
F2—C16	1.3439 (14)	C8—C9	1.3249 (16)
F3—C16	1.3301 (14)	C8—H8	0.9500

O1—C7	1.2244 (14)	C9—C10	1.4715 (16)
C1—C2	1.3802 (17)	C9—H9	0.9500
C1—C6	1.3981 (16)	C10—C11	1.3946 (16)
C1—H1	0.9500	C10—C15	1.3967 (16)
C2—C3	1.3815 (17)	C11—C12	1.3866 (16)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.3889 (17)	C12—C13	1.3874 (16)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.3850 (16)	C13—C14	1.3914 (15)
C4—H4	0.9500	C13—C16	1.4920 (16)
C5—C6	1.3929 (16)	C14—C15	1.3860 (16)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.4897 (16)	C15—H15	0.9500
C2—C1—C6	120.29 (12)	C10—C9—H9	116.1
C2—C1—H1	119.9	C11—C10—C15	118.58 (11)
C6—C1—H1	119.9	C11—C10—C9	117.90 (11)
C1—C2—C3	119.95 (12)	C15—C10—C9	123.42 (11)
C1—C2—H2	120.0	C12—C11—C10	121.06 (11)
C3—C2—H2	120.0	C12—C11—H11	119.5
C2—C3—C4	120.34 (12)	C10—C11—H11	119.5
C2—C3—H3	119.8	C11—C12—C13	119.55 (11)
C4—C3—H3	119.8	C11—C12—H12	120.2
C5—C4—C3	119.98 (12)	C13—C12—H12	120.2
C5—C4—H4	120.0	C12—C13—C14	120.32 (11)
C3—C4—H4	120.0	C12—C13—C16	119.73 (11)
C4—C5—C6	119.99 (11)	C14—C13—C16	119.94 (11)
C4—C5—H5	120.0	C15—C14—C13	119.70 (11)
C6—C5—H5	120.0	C15—C14—H14	120.1
C5—C6—C1	119.43 (11)	C13—C14—H14	120.1
C5—C6—C7	122.13 (11)	C14—C15—C10	120.78 (11)
C1—C6—C7	118.44 (11)	C14—C15—H15	119.6
O1—C7—C8	121.12 (11)	C10—C15—H15	119.6
O1—C7—C6	120.32 (11)	F3—C16—F1	106.62 (10)
C8—C7—C6	118.56 (11)	F3—C16—F2	105.91 (10)
C9—C8—C7	119.56 (11)	F1—C16—F2	105.12 (9)
C9—C8—H8	120.2	F3—C16—C13	113.26 (10)
C7—C8—H8	120.2	F1—C16—C13	113.02 (10)
C8—C9—C10	127.71 (12)	F2—C16—C13	112.27 (10)
C8—C9—H9	116.1		
C6—C1—C2—C3	−0.92 (17)	C15—C10—C11—C12	−0.73 (17)
C1—C2—C3—C4	0.55 (17)	C9—C10—C11—C12	175.76 (10)
C2—C3—C4—C5	0.65 (17)	C10—C11—C12—C13	−0.31 (17)
C3—C4—C5—C6	−1.48 (17)	C11—C12—C13—C14	0.78 (17)
C4—C5—C6—C1	1.10 (17)	C11—C12—C13—C16	179.16 (10)
C4—C5—C6—C7	−178.18 (10)	C12—C13—C14—C15	−0.18 (17)
C2—C1—C6—C5	0.10 (17)	C16—C13—C14—C15	−178.57 (10)
C2—C1—C6—C7	179.41 (10)	C13—C14—C15—C10	−0.88 (16)

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C5—C6—C7—O1	158.69 (12)	C11—C10—C15—C14	1.33 (16)
C1—C6—C7—O1	−20.61 (16)	C9—C10—C15—C14	−174.95 (10)
C5—C6—C7—C8	−22.32 (16)	C12—C13—C16—F3	145.25 (11)
C1—C6—C7—C8	158.38 (10)	C14—C13—C16—F3	−36.36 (16)
O1—C7—C8—C9	−18.27 (17)	C12—C13—C16—F1	23.86 (15)
C6—C7—C8—C9	162.75 (11)	C14—C13—C16—F1	−157.75 (10)
C7—C8—C9—C10	175.00 (10)	C12—C13—C16—F2	−94.84 (13)
C8—C9—C10—C11	171.53 (11)	C14—C13—C16—F2	83.55 (13)
C8—C9—C10—C15	−12.17 (19)		

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